

Heat and Geometry: Investigating the Geometric-Phase Origin of the Phonon Thermal Hall Effect

The primary objective of the project is to provide the experimental evidence for the phonon thermal Hall effect (PTHE) in non-magnetic insulators and then to identify the microscopic mechanisms responsible for an occurrence of this phenomenon. The thermal Hall effect (THE), historically known as the Righi-Leduc effect, manifests itself under the influence of a magnetic field as the appearance of a transverse temperature gradient in response to a longitudinal heat current. While this phenomenon was initially attributed solely to the Lorentz force acting on heat-transporting charge carriers, recently the transverse temperature gradient has been also detected in materials having only neutral mobile quasiparticles. Initial discoveries were rationalized via spin-lattice interactions or magnon-phonon hybridization but experimental evidence of large THE in simple, non-magnetic elemental crystals showed that the existing understanding is incomplete. Existing theoretical models, which rely on extrinsic scattering mechanisms or standard Berry curvature calculations within harmonic approximation, fail to reproduce the magnitude of the observed PTHE in clean materials. This suggests that a crucial ingredient is missing from currently used description of phonon dynamics in presence of a magnetic fields.

The main idea at the heart of this proposal is that the PTHE in non-magnetic insulators arises predominantly from intrinsic geometric phases acquired by phonons. We also postulate that the physical origin of this geometric phase may be distinct for different material classes. A working hypothesis assumes that in ionic insulators the dominant contribution arises from the direct action of Lorentz forces on Born effective charges. In covalent insulators, where such charges are absent, PTHE stems from the lattice Aharonov-Bohm effect. This mechanism is based on the breakdown of the adiabatic Born-Oppenheimer approximation, allowing the external magnetic field to couple with the vibrations of the crystal lattice through the electron cloud. If the position of the centre of mass of electrons is not identical to the corresponding position of the ions, an additional Berry phase is added to the phonon wave function. As a result, the outcome of phonon-phonon scattering processes becomes sensitive to the magnetic field.

The project employs a synergistic approach combining high-precision experimental measurements with advanced ab initio theoretical calculations. Experimentally, the research will investigate a broad spectrum of model insulating materials characterized by high crystalline symmetry but differing in bonding nature and defect density. The target materials include ionic and covalent binaries, but also compounds with chiral symmetry. Due to the minute magnitude of the transverse signal in non-magnetic systems, the project involves the design and construction of a specialized experimental rig. The setup is created to enable precise adjustment of the angle between the thermal gradient and the magnetic field vector, enabling comprehensive symmetry testing. On the theoretical side, the project will utilize density functional theory (DFT) and employ the direct force constant approach. To model phonon behavior at finite temperatures we will employ the high efficiency configuration space sampling (HECSS) method. A key innovation will be the integration of non-adiabatic terms to calculate the field-induced geometric phases. The research will aim to reproduce the experimental thermal Hall conductivity values by incorporating higher-order anharmonic force constants and analysing topological features, such as the phonon Berry curvature and the emergence of chiral phonons.

The scientific significance of the project is far-reaching. By establishing the intrinsic phononic origin of THE, the research will significantly contribute to an intense debate regarding heat transport in complex quantum systems. These for example include materials hosting Kitaev spin liquids or high-temperature superconductivity. Possibly, we will be able to demonstrate whether the reported transport phenomena are instead a manifestation of the ubiquitous geometric phase of phonons. The successful execution of this research and the quantitative validation of the geometric phase hypothesis in non-magnetic insulating solids, will fundamentally alter the understanding of the phononic heat transport in presence of a magnetic field.